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TITLE OF THE INVENTION (280 characters max)

MINIMUM ENERGY PULSE SYNTHESIS VIA THE INVERSE SCATTERING TRANSFORM

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Minimum Energy Pulse Synthesis via the Inverse Scattering Transform

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Abstract

This paper considers a variety of problems in the design of selective RF-pulses. We apply a formula of Faddeev and Zakharov to directly relate the energy of an RF-envelope to the magnetization profile and certain auxiliary parameters used in the inverse scattering transform approach to RF-pulse synthesis. This allows a determination of the minimum possible energy for a given magnetization profile. We give an algorithm to construct the minimum energy RF-envelope which includes an algorithm for solving the Gel'fand-Levitan-Marchenko equations.

Contents

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Introduction

The design of RF pulse sequences to produce selective excitation is a problem of principal importance in all applications of nuclear magnetic resonance. The oldest method of pulse synthesis is the *Fourier transform* method. Notwithstanding the fact that this method is an approximation for all non-zero flip angles, it gives surprising good results for flip angles up to about $\frac{\pi}{2}$. Over the past fifteen years two, more exact approaches to solving this problem have been introduced and explored. The slightly older, generally accepted method is the *Shinnar-Le Roux* or *SLR* algorithm introduced independently by M. Shinnar and his co-workers and P. Le Roux. See for example [15], [16], or [12]. A more complete list of the original papers can be found in the references to [10]. The second method is to use the *inverse scattering transform* or *IST* which was first introduced as a technique for pulse synthesis in [8] and later refined in [11, 5, 6].

From the practical perspective either method of pulse synthesis is rather demanding and requires considerable computation. From the theoretical perspective the problem of pulse synthesis is very easy. Indeed, it is clear from the inverse scattering approach that there is an *infinite dimensional* space of RF-envelopes that will produce any desired magnetization. The "real" problem of pulse synthesis is therefore to find an "optimal" RF-envelope to produce a given magnetization profile. In this paper we explore the IST approach and show how it can be used to design RF-envelopes which utilize the minimum possible energy for a given magnetization profile. At the center of our discussion is a formula expressing the energy in the RF-envelope explicitly in terms of the magnetization profile and certain *free* parameters that arise in the IST method. Formulæ of this type were discovered, in the context of inverse scattering for the Korteweg de Vries equation, by Zakharov and Faddeev in 1971! See [19]. The formula we use appears in a 1974 paper of Zakharov and Manakov, see [20]. This formula is useful both for the design of pulse sequences as well as for their analysis, as it allows for an *a posteriori* determination of the efficiency of a pulse sequence.

Underlying the derivation of the SLR algorithm is the so called *hard pulse approximation*. One designs a pulse envelope that is a finite sum of δ-pulses which produces an approximation to the desired magnetization profile. As δ-pulses are non-physical, requiring infinite energy, an SLR pulse envelope is implemented by replacing the train of δ-pulses by a train of boxcar pulses. The IST algorithm instead constructs a smooth pulse envelope which again produces an approximation to the desired magnetization profile. While such pulses are again implemented as a finite train of boxcar pulses, the approximations used in the IST are far less singular than those used in the SLR. Indeed the IST provides more direct and greater control over the final pulse envelope than

the SLR. When I undertook this work the central mystery for me was why Shinnar-Le Roux has remained the industry standard and the inverse scattering transform is largely ignored. In addition to presenting the results, which seem interesting in and of themselves, my second purpose in writing this paper is to present the IST approach in a more explicit and *palatable* form. This accounts, in part, for the somewhat expository nature of our presentation.

In the first and second sections we recall the connection between the Bloch equation without relaxation and their spin domain formulation. In inverse scattering the spin domain Bloch equation is called the Zakharov-Shabbat 2×2-system or *ZS*-system. We next review the scattering theory for the ZS-system and relate the scattering data to the magnetization profile. These sections closely follow [11], [10] and [1]. In the third section we outline the inverse scattering transform via the Gel'fand-Levitan-Marchenko equation, or more briefly the Marchenko equation, following the treatment in [1]. In the fourth section we state the formula relating the energy in the RF-envelope to the magnetization profile and the location of the bound states. In the fifth section we discuss the problem of implementing the IST. Under simplifying assumptions, we give a practical algorithm for solving the Marchenko equation. These assumptions are removed in Appendix A, where a modified algorithm is given which applies in all cases. In the sixth section we address the problem of rephasing and the physical significance of the time parameter. The seventh section contains several examples. In the eighth section we analyze the approximations used in both the SLR and IST approaches. Proofs of several mathematical results are contained in Appendix B.

1 The spin domain Bloch equation and the problem of RF-pulse synthesis

The Bloch equation without relaxation is usually written in the form

$$\frac{dM}{dt} = \gamma M \times B. \tag{1}$$

Here M is the magnetization, B is the applied magnetic field, t is time and γ is the gyromagnetic ratio. Since a vector evolves with constant length under this equation, the fundamental solution $U_0(t)$ can be regarded as $SO(3)$-valued function of time. Here we normalize so that $U_0(0)$ is Id_3, the 3×3 identity matrix. If $M(0) = M_0$ then $M(t) = U_0(t)M_0$. The solution to the Bloch equation is linear in the initial data. Throughout this paper we assume that solutions of the Bloch equation are normalized to have length equal to one.

The Bloch equation is usually analyzed in a "rotating reference" frame. Ordinarily the rotating reference frame is related to the "laboratory frame" by a time dependent orthogonal transformation of the form

$$F(t) = \begin{bmatrix} \cos\theta(t) & -\sin\theta(t) & 0 \\ \sin\theta(t) & \cos\theta(t) & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

so that

$$M(t) = F(t)m(t). \tag{2}$$

We use m to denote the magnetization in the rotating reference frame. Larmor's theorem implies that if M satisfies (1) then m satisfies

$$\frac{dm}{dt} = \gamma m \times B_{\text{eff}} \tag{3}$$

where

$$B_{\text{eff}}(t) = F^{-1}(t)B(t) + \frac{1}{\gamma}\Omega(t) \text{ with } \Omega(t) = [0, 0, \theta'(t)]^{\dagger}. \tag{4}$$

Notational remark: Most of the vectors used in this paper are to be thought of a column vectors. The notation $[a, b, c]^{\dagger}$ refers to the transpose of the row vector which is therefore a column vector, i.e.

$$[a, b, c]^{\dagger} = \begin{bmatrix} a \\ b \\ c \end{bmatrix}.$$

In most applications of this method the function $\theta(t)$ is selected to render the z-component of B_{eff} independent of time,

$$B_{\text{eff}}(f; t) = (\omega_1(t), \omega_2(t), \gamma^{-1} f). \tag{5}$$

The constant value f is called the *offset frequency* or *resonance offset*. If we set $\tilde{\omega}(t) = \omega_1(t) + i\omega_2(t)$ then, in the laboratory frame, the RF-envelope takes the form:

$$p(t) = [\operatorname{Re}\tilde{\omega}(t)e^{i\theta(t)}, \operatorname{Im}\tilde{\omega}(t)e^{i\theta(t)}, 0]^{\dagger}.$$

The energy in the RF-envelope is given by

$$W_p = \int_{-\infty}^{\infty} |p(t)|^2 dt = \int_{-\infty}^{\infty} |\tilde{\omega}(t)|^2 dt. \tag{6}$$

The magnetization profile is a unit vector valued function defined for $f \in \mathbb{R}$,

$$m^{\infty}(f) = \begin{bmatrix} m_1^{\infty}(f) \\ m_2^{\infty}(f) \\ m_3^{\infty}(f) \end{bmatrix}.$$

In essentially all MR applications $m^{\infty}(f) = [0, 0, 1]^{\dagger}$ for f outside of a bounded interval. The problem of RF-pulse synthesis is to find a time dependent complex pulse envelope $\tilde{\omega}(t)$ so that, if $B_{\text{eff}}(f)$ is given by (5), then the solution of

$$\frac{dm}{dt}(f; t) = \gamma m(f; t) \times B_{\text{eff}}(f; t) \tag{7}$$

with

$$\lim_{t \to -\infty} m(f; t) = [0, 0, 1]^{\dagger} \tag{8}$$

satisfies

$$\lim_{t \to \infty} [e^{-ift}(m_1 + im_2)(f; t), m_3(f; t)] = [(m_1^{\infty} + im_2^{\infty})(f), m_3^{\infty}(f)]. \tag{9}$$

We have used the standard complex notation for the transverse components of the magnetization. If $\tilde{\omega}$ is supported in the interval $[t_0, t_1]$ then these asymptotic conditions are replaced by

$$\begin{gathered} m(f; t_0) = [0, 0, 1]^{\dagger}, \\ [e^{-ift_1}(m_1 + im_2)(f; t_1), m_3(f; t_1)] = [(m_1^{\infty} + im_2^{\infty})(f), m_3^{\infty}(f)]. \end{gathered} \tag{10}$$

The mapping from ω to m^{∞} is highly non-linear.

To solve the problem of RF-pulse synthesis it is convenient to introduce the spin domain formulation of the Bloch equation. Instead of a unit vector m in $\mathbb{R}^3$ we solve for a unit vector ψ in $\mathbb{C}^2$. This vector satisfies the 2×2 matrix equation:

$$\frac{d\psi}{dt} = -\frac{i}{2} \Omega \cdot \sigma \psi. \tag{11}$$

Here $\Omega = -[\gamma\omega_1(t), \gamma\omega_2(t), f]$ and σ are the Pauli spin matrices:

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Assembling the pieces we see that ψ satisfies[1]

$$\frac{d\psi}{dt}(\xi; t) = \begin{bmatrix} -i\xi & q(t) \\ -q^*(t) & i\xi \end{bmatrix} \psi(\xi; t), \tag{12}$$

with

$$\xi = \frac{f}{2}, \quad q = \frac{-i\gamma}{2}(\omega_1(t) - i\omega_2(t)).$$

A simple recipe takes a solution of (12) and produces a solution of (7). If $\psi(\xi; t) = [\psi_1(\xi; t), \psi_2(\xi; t)]^{\dagger}$ satisfies (12) then the 3-vector

$$m(f; t) = [2\,\text{Re}(\psi_1^*\psi_2), 2\,\text{Im}(\psi_1^*\psi_2), |\psi_1|^2 - |\psi_2|^2]^{\dagger}(\frac{f}{2}; t) \tag{13}$$

[1] We follow the standard practice in the MR literature of using z^* to denote the complex conjugate of the complex number z.

satisfies (7). If in addition

$$\lim_{t\to-\infty} \psi(\xi;t) = \begin{bmatrix} e^{-i\xi t} \\ 0 \end{bmatrix}$$

then m satisfies (8). Thus the RF-pulse synthesis problem is easily translated into a inverse scattering problem for equation (12). This is described in the next section. Following the standard practice in inverse scattering we refer to equation (12) as the *ZS-system* and q as the *potential.*

2 Scattering theory for the ZS-system

Scattering theory for an equation like (12) relates the behavior of $\lim_{t\to-\infty} \psi(\xi;t)$ to that of $\lim_{t\to\infty} \psi(\xi;t)$. If q has bounded support then the functions

$$\begin{bmatrix} e^{-i\xi t} \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ e^{i\xi t} \end{bmatrix}$$

are a basis of solutions for (12) outside the support of q. If the L^1-norm of q is finite then it is shown in [1] that (12) has solutions which are asymptotic to these solutions as $t \to \pm\infty$.

Theorem 1. *If $\|q\|_{L^1}$ is finite then for every real ξ there are* unique *solutions*

$$\psi_{1+}(\xi),\ \psi_{2+}(\xi) \text{ and } \psi_{1-}(\xi),\ \psi_{2-}(\xi)$$

to equation (12) *which satisfy*

$$\lim_{t\to-\infty} e^{i\xi t}\psi_{1-}(\xi;t) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \lim_{t\to-\infty} e^{-i\xi t}\psi_{2-}(\xi;t) = \begin{bmatrix} 0 \\ -1 \end{bmatrix} \tag{14}$$

$$\lim_{t\to\infty} e^{i\xi t}\psi_{1+}(\xi;t) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \lim_{t\to\infty} e^{-i\xi t}\psi_{2+}(\xi;t) = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{15}$$

The solutions $\psi_{1-}(\xi)$, $\psi_{2+}(\xi)$ extend as analytic functions of ξ to the upper half plane, $\operatorname{Im}\xi > 0$ *and $\psi_{2-}(\xi)$, $\psi_{1+}(\xi)$ extend as analytic functions of ξ to the lower half plane,* $\operatorname{Im}\xi < 0$.

The proof of this theorem can be found in [1]. We briefly outline the construction of these solutions as we will need these formulæ later on.

Outline of proof. The idea is to re-express the boundary value problems for the differential equation as Volterra integral equations. Let

$$\psi_{1-} = \begin{bmatrix} \psi_{11-} \\ \psi_{21-} \end{bmatrix}, \quad \psi_{2-} = \begin{bmatrix} \psi_{12-} \\ \psi_{22-} \end{bmatrix}.$$

These solutions satisfy:

$$\begin{aligned}
\psi_{11-}(\xi;t)e^{i\xi t} &= 1+\int_{-\infty}^{t} M_1(\xi;t,s)\psi_{11-}(\xi;s)e^{i\xi s}ds,\\
\psi_{21-}(\xi;t)e^{i\xi t} &= -\int_{-\infty}^{t} e^{2i\xi(t-s)}q^*(s)\psi_{11-}(\xi;s)e^{i\xi s}ds,\\
\psi_{22-}(\xi;t)e^{-i\xi t} &= -1+\int_{-\infty}^{t} M_2(\xi;t,s)\psi_{22-}(\xi;s)e^{-i\xi s}ds,\\
\psi_{12-}(\xi;t)e^{-i\xi t} &= -\int_{-\infty}^{t} e^{-2i\xi(t-s)}q(s)\psi_{22-}(\xi;s)e^{-i\xi s}ds,
\end{aligned} \tag{16}$$

where

$$\begin{aligned}
M_1(\xi;t,s) &= -q^*(s)\int_{s}^{t} e^{2i\xi(x-s)}q(x)dx,\\
M_2(\xi;t,s) &= -q(s)\int_{s}^{t} e^{2i\xi(s-x)}q^*(x)dx.
\end{aligned} \tag{17}$$

The solutions normalized at $+\infty$ satisfy similar equations. If we set

$$Q_1(t) = \int_{-\infty}^{t} |q(s)|ds$$

then it is shown in [1] that these equations can be solved for ξ in the appropriate half plane by iteration and

$$|\psi_{11-}(\xi;t)e^{i\xi t}| \leq I_0(2Q_1(t)), \quad |\psi_{22-}(\xi;t)e^{-i\xi t}| \leq I_0(2Q_1(t)). \tag{18}$$

Here I_0 is the classical I_0-Bessel function. The same argument applies *mutatis mutandis* to obtain ψ_{1+} and ψ_{2+}. □

For real values of ξ the solutions normalized at $-\infty$ can be expressed in terms of the solutions normalized at $+\infty$ by the linear relations

$$\begin{aligned}
\psi_{1-}(\xi;t) &= a(\xi)\psi_{1+}(\xi;t)+b(\xi)\psi_{2+}(\xi;t),\\
\psi_{2-}(\xi;t) &= b^*(\xi)\psi_{1+}(\xi;t)-a^*(\xi)\psi_{2+}(\xi;t).
\end{aligned} \tag{19}$$

The functions a, b are called the *scattering coefficients* for the potential q. The 2×2-matrices $[\psi_{1-}\psi_{2-}]$, $[\psi_{1+}\psi_{2+}]$ satisfy

$$[\psi_{1-}\psi_{2-}] = [\psi_{1+}\psi_{2+}]\begin{bmatrix} a(\xi) & b^*(\xi)\\ b(\xi) & -a^*(\xi)\end{bmatrix}. \tag{20}$$

The *scattering matrix* for the potential q is defined to be

$$s(\xi) = \begin{bmatrix} a(\xi) & b^*(\xi) \\ b(\xi) & -a^*(\xi) \end{bmatrix}. \tag{21}$$

Recall that the *Wronskian* between two $\mathbb{C}^2$-valued functions is defined by

$$W(u, v)(t) \stackrel{d}{=} u_1(t)v_2(t) - u_2(t)v_1(t).$$

If $u(t)$ and $v(t)$ are solutions of (12), for the same value of ξ, then $W(u(t), v(t))$ is independent of t. It is not difficult to show that

$$\begin{aligned} a(\xi) &= [\psi_{11-}(\xi;t)\psi_{22+}(\xi;t) - \psi_{21-}(\xi;t)\psi_{12+}(\xi;t)] = W(\psi_{1-}, \psi_{2+})(t), \\ b(\xi) &= -[\psi_{11-}(\xi;t)\psi_{21+}(\xi;t) - \psi_{21-}(\xi;t)\psi_{11+}(\xi;t)] = -W(\psi_{1-}, \psi_{1+})(t). \end{aligned} \tag{22}$$

It follows from (22) that a extends to the upper half plane as an analytic function. If q has an integrable derivative then, using (16) and (22) it can be shown that

$$a(\xi) = 1 + \frac{1}{2i\xi} \int_{-\infty}^{\infty} |q(s)|^2 ds + O(\frac{1}{\xi^2}) \tag{23}$$

as $|\xi|$ tends to infinity in $\operatorname{Im}\xi \geq 0$. As $W(\psi_{1-}, \psi_{2-}) = -1$ it follows that

$$|a(\xi)|^2 + |b(\xi)|^2 = 1, \tag{24}$$

and therefore (23) implies that

$$|b(\xi)| = O(\frac{1}{|\xi|}) \text{ as } \xi \to \pm\infty. \tag{25}$$

These results are proved in [1].

Assuming that $t^j q(t)$ is integrable for all j it is shown in [1] that a has finitely many zeros in $\operatorname{Im}\xi \geq 0$. Let $\{\xi_1, \ldots, \xi_N\}$ be a list of the zeros of a. For each j it follows from (22) that there is a *non-zero* complex number C_j so that

$$\psi_{1-}(\xi_j) = C_j \psi_{2+}(\xi_j), \quad j = 1, \ldots, N. \tag{26}$$

The constants $\{C_1, \ldots, C_N\}$ appearing in (26) are called *norming constants*. Equation (12) can be rewritten in the form

$$\begin{bmatrix} i\partial_t & -iq \\ -iq^* & -i\partial_t \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \xi \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}. \tag{27}$$

From this formulation it is clear that ξ should be regarded as a spectral parameter. If ξ has positive imaginary part then $\psi_{1-}(\xi;t)$ decays exponentially as t tends to $-\infty$ and $\psi_{2+}(\xi;t)$ decays exponentially as t tends to $+\infty$. If $a(\xi_j) = 0$ then (26) implies that $\psi_{1-}(\xi_j;t)$ decays exponentially at both $\pm\infty$ and therefore the function $\psi_{1-}(\xi_j;t)$

belongs to $L^2(\mathbb{R};\mathbb{C}^2)$. Thus the operator on the left hand side of (27) has *bound states* for these values of the offset frequency.

We generally assume that the zeros of a are simple and that their imaginary parts are positive. This is mostly to simplify the exposition, there is no difficulty, in principle, if a has real zeros or higher order zeros. Using the argument principle and (23) it follows that

$$N = \frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{a'(\xi)d\xi}{a(\xi)}. \tag{28}$$

Definition 1. The pair of functions $(a(\xi), b(\xi))$, for $\xi \in \mathbb{R}$ and the collection of pairs $\{(\xi_j, C_j) : j = 1, \ldots, N\}$ define the *scattering data* for equation (12).

The scattering data are not quite independent. Since a is analytic in the upper half plane it follows from (24) and (23) that, for $\operatorname{Im}\xi > 0$, we have:

$$a(\xi) = \prod_{j=1}^{N}\left(\frac{\xi - \xi_j}{\xi - \xi_j^*}\right)\exp\left[\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{\log(1 - |b(\zeta)|^2)d\zeta}{\zeta - \xi}\right]. \tag{29}$$

see [7]. The *reflection* coefficient is defined by:

$$r(\xi) = \frac{b(\xi)}{a(\xi)}; \tag{30}$$

A priori the reflection coefficient is only defined on the real axis. We rewrite (29) in terms of r :

$$a(\xi) = \prod_{j=1}^{n}\left(\frac{\xi - \xi_j}{\xi - \xi_j^*}\right)\exp\left[\frac{i}{2\pi}\int_{-\infty}^{\infty}\frac{\log(1+|r(\zeta)|^2)d\zeta}{\zeta - \xi}\right]. \tag{31}$$

Both (29) and (31) have well defined limits as ξ approaches the real axis.

Definition 2. The function $r(\xi)$, for $\xi \in \mathbb{R}$ and the collection of pairs $\{(\xi_j, C_j) : j = 1, \ldots, N\}$ define the *reduced scattering data* for equation (12).

Implicitly the reduced scattering data is a function of the potential q. In inverse scattering theory the data $\{r; (\xi_1, C_1), \ldots, (\xi_N, C_N)\}$ are specfied and we seek a potential q which has this reduced scattering data. The map from this data to q is often called the *Inverse Scattering Transform* or *IST*.

We close this section by rephrasing the RF-pulse synthesis problem as an inverse scattering problem. Recall that the data for the pulse synthesis problem is the magnetization profile m^{∞} which we now think of as a function of $\xi = f/2$. Using (13), the solution ψ_{1-}, to the ZS-system defines a solution m_{1-} to (7), satisfying (8). It follows from (15) and (19) that

$$\psi_{1-}(\xi;t) \sim \begin{bmatrix} a(\xi)e^{-i\xi t} \\ b(\xi)e^{i\xi t}\end{bmatrix} \text{ as } t \to +\infty. \tag{32}$$

Therefore

$$m_{1-}(\xi;t) \sim \begin{bmatrix} 2b(\xi)a^*(\xi)e^{2i\xi t} \\ |a(\xi)|^2 - |b(\xi)|^2 \end{bmatrix}, \tag{33}$$

where, as before, we use the complex notation for the transverse components of m_{1-}. If m_{1-} also satisfies (9) then it follows from (33) and (24) that

$$\begin{aligned} \frac{b(\xi)}{a(\xi)} &= \lim_{t\to\infty} \frac{(m_{11-}+im_{21-})(\xi;t)e^{-2i\xi t}}{1+m_{31-}(\xi;t)} \\ &= \frac{(m_1^\infty + im_2^\infty)(\xi)}{1+m_3^\infty(\xi)}. \end{aligned} \tag{34}$$

In light of this formula we sometimes refer to r as the *stereographic magnetization profile*. If q has support in the ray $(-\infty, t_1]$ then

$$r(\xi) = \frac{(m_{11-}+im_{21-})(\xi;t)e^{-2i\xi t}}{1+m_{31-}(\xi;t)} \tag{35}$$

is independent of t for $t > t_1$.

As m^∞ is a unit vector valued function we see that the reflection coefficient $r(\xi)$ uniquely determines $m^\infty(\xi)$ and vice-versa. Thus the RF-pulse synthesis problem can be rephrased as the following inverse scattering problem:

> Find a potential q for the ZS-system so that the reflection coefficient r satisfies (34) for all real ξ.

Note that the pulse synthesis problem makes no reference to the data connected to the bound states, i.e. $\{(\xi_j, C_j)\}$. Indeed these are *free* parameters in the pulse synthesis problem, making the problem higly underdetermined. Perhaps the main result of this paper is that, for a given magnetization profile, the RF-envelope requiring the minimum energy is the one for which the ZS-system has *no* bound states.

Remark 1. The material in this section is largely adapted from [1], [11] and [10].

3 Inverse scattering for the ZS-equation

There are several different approaches to solving the inverse scattering problem stated at the end of the previous section, see [1], [2], [4] or [7]. In this section we describe the solution of this problem via the Marchenko equations. We again follow the presentation in [1]. We generally suppose that the $\{\xi_j\}$ are distinct complex number with positive imaginary parts. To begin with we assume that the reflection coefficient is smooth and rapidly vanishing at $\pm\infty$. Using limiting arguments the latter restriction is easily relaxed.

The Marchenko equations are systems of integral equations of Fredholm type. Given the scattering data $\{r; (\xi_1, C_1), \ldots, (\xi_N, C_N)\}$ define the function

$$f(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} r(\xi)e^{i\xi t}d\xi - i\sum_{j=1}^{N} C_j e^{i\xi_j t}. \tag{36}$$

This is the inverse Fourier transform of r with a correction added to account for the bound states. Note that the finite sum is exponentially decreasing as t tends to $+\infty$. Define the 2×2 matrix valued function:

$$\mathcal{F}(t) = \begin{bmatrix} 0 & -f^*(t) \\ f(t) & 0 \end{bmatrix}.$$

For each number $t \in \mathbb{R}$ we seek a 2×2-matrix valued function $\mathcal{K}_t(s)$, defined for $s \in [t, \infty)$, which solves the integral equation:

$$\mathcal{K}_t(s) + \int_t^\infty \mathcal{K}_t(\sigma)\mathcal{F}(s+\sigma)d\sigma = -\mathcal{F}(t+s) \text{ for } s \in [t, \infty). \tag{37}$$

Under our assumptions on r it is not difficult to show that, for every $t \in \mathbb{R}$, (37) is a Fredholm integral equation on $L^2([t, \infty); gl_2)$. Since $\mathcal{F}(t+\cdot)$ belongs to $L^2([t, \infty); gl_2)$, the solvability of (37) follows if it can be shown that any solution to the homogeneous adjoint equation,

$$\mathcal{L}(s) + \int_t^\infty \mathcal{L}(\sigma)\mathcal{F}^*(s+\sigma)d\sigma = 0$$

is identically zero. This proof of this statement can be found in [1]. The uniqueness of the solution to (37) follows from the fact that homogeneous equation corresponding to (37) also has only the trivial solution.

Remark 2. For the theory of Fredholm integral equations see [18]. For the moment we note that the known proofs for the existence of a solution to a Fredholm equation do not generally provide a practicable algorithm to find the solution.

The connection between the inverse scattering problem and the Marchenko equation is summarized in the following theorem:

Theorem 2. *Given a smooth, rapidly decaying reflection coefficient r and a finite set of pairs $\{(\xi_j, C_j) : j = 1, \ldots, N\}$, with the $\{\xi_j\}$ distinct,* $\operatorname{Im}\xi_j > 0$ *and* $C_j \neq 0$ *for* $j = 1, \ldots, N$, *the equation* (37) *has a unique solution for every $t \in \mathbb{R}$. If*

$$q(t) = -2\mathcal{K}_{12t}(t) \tag{38}$$

then the ZS-system with this potential has reflection coefficient r. It has exactly N bound states for frequencies $\{\xi_1, \ldots, \xi_N\}$ and the relations (26) *hold at these points.*

This theorem is proved in [7] and, in a slightly different formulation in [2].

Remark 3. As noted above, there is a similar result if a has higher order zeros or zeros on the real line. In this case the definition of f needs to be modified, we return to this in Appendix A.

We defer a discussion of the practicalities of solving (37) to section 5. For the moment suffice it to say that this equation can be solved by a simple iteration for values of t such that

$$\int_{2t}^\infty \|\mathcal{F}(\sigma)\|d\sigma < 1,$$

while a somewhat indirect method is required for smaller values of t. There is also "left" Marchenko equation, given in section 5, where the integrals are over half lines of the form $(-\infty, t]$. In this formulation the finite sum of exponentials is decreasing as t tends to $-\infty$.

The regularity and decay of q are related to the regularity and decay of r exactly as if they were a Fourier transform pair. The following result is a special case of a theorem proved in [2]:

Theorem 3 (Beals-Coifman). *Suppose that r is a reflection coefficient and q is the corresponding potential for the ZS-system. Let k be a positive integer.*

1. *If*
$$\int_{-\infty}^{\infty} [|\xi|^{2k} + 1]|r(\xi)|^2 d\xi < \infty$$
then the distributional derivatives $\partial_t^j q$ for $0 \leq j \leq k$ belong to $L^2(\mathbb{R}) + L^\infty(\mathbb{R})$.

2. *If the distribution derivatives $\partial_\xi^j r \in L^2(\mathbb{R})$ for $0 < j \leq k+1$ then $t^{k+1} q \in L^2(\mathbb{R}) + L^\infty(\mathbb{R})$.*

Remark 4. There are no smallness hypotheses in this theorem. Note also that this theorem does not mention the bound states. While the bound states exercise a strong effect on the detailed structure of q, their presence or absence has no effect on the gross smoothness and decay properties of the potential. These features of q are governed entirely by the reflection coefficient.

Remark 5. It has been noted many times in both the inverse scattering and MR literatures that, as q tends to zero, $r^*(\xi)$ tends to $\hat{q}(-2\xi)$. The results of Beals and Coifman shows that the connection between the inverse scattering transform and the Fourier transform is much deeper than that previously described. There is also an analogue of the Paley-Wiener theorem (see Appendix B): If the reflection coefficient has bounded support then the potential does not. This is easier to see in the logically equivalent contrapositive form: If the potential has bounded support then the reflection coefficient does not. When the potential has bounded support the scattering coefficients (a, b) extend, as analytic functions, to the entire complex plane. This means that the set where b and therefore r vanishes is discrete. Hence the reflection coefficient, restricted to the real axis, cannot have bounded support.

Remark 6. Beals and Coifman show that the IST can be extended to square integrable reflection coefficients such that $\partial_\xi r$ also belongs to $L^2(\mathbb{R})$. By using smooth, compactly support approximating sequences, the estimates in the theorem can be extended to data with finitely many derivatives and finite rates of decay.

The results of this section show that, at least in principle, the IST provides many solutions to the RF-pulse synthesis problem. A practical magnetization profile has bounded support and may be approximated by a smooth function. This leaves two essential problems:

1. Given m^{∞} (and therefore r) how should the bound states be selected to give an "optimal" RF-pulse envelope which will produce the desired magnetization profile?

2. How is the Marchenko equation to be solved?

The notion of optimality depends on the intended application. It usually entails a balance among the energy, duration, oscillation and need for rephasing of the RF-envelope. In the remainder of the paper we focus on the construction of the minimum energy RF-envelope.

4 The energy of the RF-envelope

We now state a formula for the energy of the pulse envelope in terms of the scattering data. The underlying results are due to Zakharov, Faddeev and Manakov.

Theorem 4. *Suppose that q is a sufficiently rapidly decaying potential for the ZS-system with reflection coefficient r and discrete data $\{(\xi_j, C_j), j = 1, \ldots, N\}$ then*

$$\int_{-\infty}^{\infty} |q(t)|^2 dt = \frac{1}{\pi} \int_{-\infty}^{\infty} \log(1 + |r(\xi)|^2) d\xi + 4 \sum_{j=1}^{N} \operatorname{Im} \xi_j. \tag{39}$$

The proof of this result can be found in [1] or [7]. Note that the norming constants play no role in this formula. Formula (39) is just one from an infinite sequence of formulæ relating functionals of the potential to functionals of the reduced scattering data.

Combining (6), (39) with (34) we obtain the following simple corollary.

Corollary 1. *If m^{∞} is a sufficiently smooth magnetization profile such that $m_1^{\infty} + i m_2^{\infty}$ vanishes outside a finite interval then the total energy of any RF-envelope ω which produces this magnetization profile satisfies the estimate*

$$\int_{-\infty}^{\infty} |\omega(t)|^2 dt \geq \frac{2}{\pi \gamma^2} \int \log\left(1 + \left|\frac{m_1^{\infty}(\xi) + i m_2^{\infty}(\xi)}{1 + m_3^{\infty}(\xi)}\right|^2\right) d\xi. \tag{40}$$

Equality holds in this estimate if and only if the ZS-system with the corresponding potential has no bound states.

From the corollary it is evident that the lowest energy RF-envelope is obtained by solving the Marchenko equation with

$$f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} r(\xi) e^{i\xi t} d\xi.$$

Remark 7. There are several other immediate conclusions which can be drawn from this formula. Often times one seeks to specify a particular dependence for the phase of the transverse magnetization. Changing the phase of the transverse magnetization amounts to replacing $(m_1^\infty(\xi) + im_2^\infty(\xi))$ by $(m_1^\infty(\xi) + im_2^\infty(\xi))e^{i\phi(\xi)}$, where ϕ is a real valued function. From (40) it is apparent that the energy required for the minimum energy RF-envelope is independent of the phase of the transverse magnetization. Note however that the minimum energy pulse will in general require rephasing. This is addressed in section 6.

Remark 8. Very important types of pulses in MR imaging are inversion or refocussing pulses. Such a pulse carries $[0, 0, 1]$ to $[0, 0, -1]$. If this is the case at offset frequency ξ then $r(\xi) = \infty$. It would therefore require infinite energy to exactly invert $[0, 0, 1]$ for offset frequencies belonging to an interval of positive length. The energy required to carry $[0, 0, 1]$ to a vector of the form $[m_1, m_2, -1 + e]$ for $0 \leq e < \epsilon$ and offset frequencies belonging to a band of width B, is at least

$$\frac{2B}{\pi\gamma^2}\log\left(1 + \frac{4(2-\epsilon)}{\epsilon}\right).$$

Ideally we would like to have a functional that estimates the support of q in terms of the scattering data. An explicit formula of this sort has proved elusive. On the other hand, as we shall see in section 5, the Marchenko equation implies that the *effective* support of q is largely determined by the effective support of the function f defined in (36).

In the absence of bound states it is not hard to show that if $r(\xi)$ is the reflection coefficient determined by $q(t)$ then $r(\lambda\xi)$ comes from the potential $\lambda^{-1}q(\lambda^{-1}t)$. This agrees with the well known heuristic principle that the effective support of the RF-envelope is inversely proportional to the bandwidth of excitation. It also shows that the maximum amplitude and energy of the RF-envelope are proportional to the bandwidth. The L^2-oscillation of the RF-envelope, $\int |q_t|^2 dt$, is proportional to the square of the bandwidth.

5 Solving the Marchenko equation with no bound states

In this section we discuss an algorithmic approach for obtaining the minimum energy RF-envelope. It entails solving the Marchenko equation, (37) and a related equation, (42) given below. Our method involves solving the Marchenko equations directly via iteration. As noted above, this requires some care as large data may lead to a divergent series. In [11] Rourke and Morris introduced a method for solving the Marchenko equation by adapting a method of Moses and Proesser, see [9]. The analysis in [11] differs in one small particular from that in [9], leading to solutions of the Marchenko equation with non-trivial bound states and therefore sub-optimal energy requirement.

The method of Moses and Proesser is to approximate the reflection coefficient by a rational function with all of it poles *in the lower half plane*. This ensures that the resultant potential is supported in $(-\infty, 0]$ and has no bound states. In [11] this condition on the placement of the poles is not respected. Indeed in examples 2 and 3 of [11]

they use a rational approximation to r with poles in both half planes; the solutions they found were supported in a proper subinterval of $(-\infty, 0)$. However the poles of r in the upper half plane force the resultant potential for the ZS-system to have non-trivial bound states. These increase the needed energy and oscillation without affecting the magnetization profile. Regrettably the method of Moses and Proesser is not generally applicable to find the minimum energy RF-envelope. This is due to the well known consequence of the maximum principle in the theory of functions of a complex variable: A function on the real line which tends to zero at infinity is only well approximated by rational functions with poles in the lower half plane if it is the boundary value of an analytic function defined in the upper half plane. In light of a classical theorem of Fatou, this excludes any function supported in a bounded interval, see [13].

We are left with little choice but to solve the Marchenko equation directly. We now present an algorithm for doing this. The algorithm is described in the realm of continuum mathematics but can easily be approximately implemented on a computer. We will return to the question of implementation in a later publication. After stating the "left" Marchenko equation we give an estimate which shows that, for a given reflection coefficient, the Marchenko equations can be solved for sufficienty large $|t|$. There are two ideas which underlie our algorithm:

1. Using the Marchenko equation we solve for the potential *one t at a time*.
2. If $q = q_1 + q_2$ where q_1 and q_2 have disjoint supports then the scattering data for q has a simple, explicit expression in terms of the scattering data for q_1 and q_2.

Using these ideas leads to a method which allows us to work inward from $\pm\infty$ to determine the potential for all values of t.

Theorem 2 and its extension to less regular data imply that, given a sufficiently regular reflection coefficient r, there exists a potential q so that the ZS-system, with this potential, has reflection coefficient r and no bound states. In this and the following section the data r and the corresponding potential q are fixed. We assume that r decays rapidly enough and is sufficiently regular for q to be bounded and integrable with two continuous derivatives, see Theorem 3.

Equation (37) involves integration over positive half rays. Because of the divergences indicated above it is useful to work both ends against the middle. For that purpose we give the *left Marchenko equation* which involves integration over negative half rays. For later applications we give the left Marchenko equation with finitely many bound states. Recall that $r = b/a$; given r we can use (31) to determine a and therefore b. Define

$$\tilde{r}(\xi) = \frac{b^*(\xi)}{a(\xi)}$$

and let $\{\xi_1, \dots, \xi_N\}$ be points in the upper half plane. There are non-zero constants $\{\widetilde{C}_j\}$ so that the kernel function for the left Marchenko equation is defined by

$$g(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \tilde{r}(\xi)e^{-i\xi t}dt - i\sum_{j=1}^{N}\widetilde{C}_j e^{-i\xi_j^* t} \tag{41}$$

The exponential correction terms are exponentially decaying as t tends to $-\infty$. The kernel for the left Marchenko equation is

$$\mathcal{G}(t) = \begin{bmatrix} 0 & g(t) \\ -g^*(t) & 0 \end{bmatrix}.$$

For each fixed $t \in \mathbb{R}$ the equation is

$$\mathcal{L}_t(s) + \int_{-\infty}^{t} \mathcal{L}_t(x)\mathcal{G}(x+s)dx = -\mathcal{G}(t+s) \text{ for } s \in (-\infty, t]. \tag{42}$$

If $\mathcal{L}_t(s)$ solves this equation then the potential defined by

$$q(t) = 2\mathcal{L}_t(t)$$

has reflection coefficient r and bound states at $\{\xi_j\}$. In the remainder of our analysis we concentrate on the "right" Marchenko equation, (37), with the understanding that everything said applies *mutatis mutandis* to the left formulation as well.

Let $|||\cdot|||$ denote an operator norm on 2×2-matrices; this means that $|||\cdot|||$ is a norm which satisfies:

$$|||AB||| \leq |||A|||\,|||B|||$$

For example we can take

$$|||A||| = \max_{v \neq 0} \frac{\|Av\|}{\|v\|}.$$

Define the functions

$$M_f(t) = \sup_{s \geq t} |||\mathcal{F}(s)|||,$$
$$I_f(t) = \int_t^{\infty} |||\mathcal{F}(s)|||\, ds. \tag{43}$$

We say that the Marchenko equation can be *solved by iteration* on the interval $[t, \infty)$ if the sequence defined by

$$\mathcal{K}_t^0(s) = -\mathcal{F}(s+t),$$
$$\mathcal{K}_t^j(s) = -\mathcal{F}(s+t) + \int_t^{\infty} \mathcal{K}_t^{j-1}(s+x)\mathcal{F}(t+x)dx, \quad j = 1, 2, \ldots \tag{44}$$

converges uniformly to $\mathcal{K}_t(s)$ for $s \in [t, \infty)$.

Theorem 5. *If $I_f(2t) < 1$ then the Marchenko equation can be solved by iteration on the interval $[t, \infty)$. The solution satisfies the estimate*

$$\mathcal{K}_t(s) \leq \frac{M_f(t+s)}{1 - I_f(2t)}. \tag{45}$$

The proof is given in Appendix B. Note that no assumption is made here about the presence or absence of bound states.

The estimate (45) implies that, so long as the hypotheses of the theorem hold, the potential q satisfies the estimate

$$|q(t)| \leq \frac{2M_f(2t)}{1 - I_f(2t)}. \tag{46}$$

This in turn explains our claim that the essential support of q is determined by the essential support of f. A similar result holds for the left Marchenko equation. Taken together they show that if r decays rapidly enough and is sufficiently smooth then the potential q can be determined, by iteration outside of a bounded interval $[t_-, t_+]$. If $I_f(-\infty) < 2$ then q can be determined on the whole real line by iteration.

If $I_f(-\infty) \geq 2$ then an additional trick may be needed. If we rewrite the potential q as a sum of potentials with disjoint support:

$$\begin{aligned} q &= \chi_{(-\infty,t_0]}q + \chi_{(t_0,\infty]}q \\ &= q_1 + q_2 \end{aligned} \tag{47}$$

then the scattering matrix of q is easily expressed in terms of the scattering matrices of q_1 and q_2. Indeed we have two formulæ.

Theorem 6. *Suppose that $q = q_1 + q_2$ where the support of q_1 is to the left of the support of q_2. If*

$$s_i = \begin{bmatrix} a_i & b_i^* \\ b_i & -a_i^* \end{bmatrix}, \quad i = 1, 2,$$

are the scattering matrices defined by q_i, $i = 1, 2$, respectively then the scattering matrix defined by q is given by

$$\begin{aligned} \begin{bmatrix} a & b^* \\ b & -a^* \end{bmatrix} &= \begin{bmatrix} a_2 & -b_2^* \\ b_2 & a_2^* \end{bmatrix} \begin{bmatrix} a_1 & b_1^* \\ b_1 & -a_1^* \end{bmatrix} \\ &= \begin{bmatrix} a_2 & b_2^* \\ b_2 & -a_2^* \end{bmatrix} \begin{bmatrix} a_1 & b_1^* \\ -b_1 & a_1^* \end{bmatrix} \end{aligned} \tag{48}$$

These formulæ are elementary consequences of the definition of the scattering matrix.

The abstract existence theory for the Marchenko equation assures that, given a sufficiently smooth, square integrable reflection coefficient r, there are solutions of the corresponding Marchenko equations for every $t \in \mathbb{R}$ and therefore a potential q which defines a ZS-system with no bound states and the given reflection coefficient. In light of Theorem 5 there are numbers $\{t_-^{(0)}, t_+^{(0)}\}$ so that we can solve the left and right Marchenko equations by iteration to find

$$\begin{aligned} q_-^{(0)} &= \chi_{(-\infty,t_-^{(0)}]}q \text{ and} \\ q_+^{(0)} &= \chi_{[t_+^{(0)},\infty)}q. \end{aligned} \tag{49}$$

If $t_-^{(0)} \geq t_+^{(0)}$ then we are done. Otherwise we need to solve the forward scattering problem for the potentials $q_-^{(0)}$ and $q_+^{(0)}$ to obtain the scattering coefficients $\{(a_\pm^{(0)}, b_\pm^{(0)})\}$. Using Theorem 6 twice we obtain the relation:

$$\begin{bmatrix} a & b^* \\ b & -a^* \end{bmatrix} = \begin{bmatrix} a_+^{(0)*} & -b_+^{(0)*} \\ b_+^{(0)} & a_+^{(0)*} \end{bmatrix} \begin{bmatrix} a_1 & b_1^* \\ b_1 & -a_1^* \end{bmatrix} \begin{bmatrix} a_-^{(0)} & b_-^{(0)*} \\ -b_-^{(0)} & a_-^{(0)*} \end{bmatrix}. \tag{50}$$

Here (a_1, b_1) are the scattering coefficients for the (unknown part of the) potential

$$q_1 = \chi_{[t_-^{(0)}, t_+^{(0)}]} q. \tag{51}$$

Using (50) we solve for the scattering coefficients of q_1. Since q_1 is a potential with bounded support the functions (a_1, b_1) extend as analytic functions to the entire complex plane. It is not clear whether or not the ZS-system with potential q_1 has any bound states. In fact our algorithm applies in either case. To simplify the exposition we assume, for now, that for all $\alpha < \beta$ the potentials $\chi_{[\alpha,\beta]} q$ have no bound states. In Appendix A we explain how to remove this hypothesis. The iterative step in the algorithm relies on the following Paley-Wiener type theorem:

Theorem 7. *Suppose that q is a potential for the ZS-system with support in the half line $(-\infty, t_+]$ ($[t_-, \infty)$). Then the kernel function f for the Marchenko equation, defined in (36), (g defined in (41)) is supported in the ray $(-\infty, 2t_+]$ ($[2t_-, \infty)$).*

The proof of this result is given in Appendix A.

Assuming that q_1 has no bound states, the pair of functions (a_1, b_1) is the scattering data for a potential with support in the finite interval $[t_-^{(0)}, t_+^{(0)}]$. Theorem 7 therefore applies to show that

$$f_1(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} r_1(\xi) e^{i\xi t} d\xi \tag{52}$$

is a function with support in the interval $(-\infty, 2t_+^{(0)}]$, with an analogous conclusion for g_1.

From Theorem 5 it follows that there exists another pair $(t_-^{(1)}, t_+^{(1)})$ such that

$$t_-^{(0)} < t_-^{(1)}, \quad t_+^{(1)} < t_+^{(0)}$$

and the Marchenko equations, with the kernels defined by g_1, f_1, can be solved by iteration on the intevals $(-\infty, t_-^{(1)}]$ and $[t_+^{(1)}, \infty)$ respectively. Note that the potential q is now determined on the complement of $[t_-^{(1)}, t_+^{(1)}]$. Next the scattering data for the potentials

$$\begin{aligned} q_-^{(1)} &= \chi_{[t_-^{(0)}, t_-^{(1)}]} q \text{ and} \\ q_+^{(0)} &= \chi_{[t_+^{(1)}, t_+^{(0)}]} q. \end{aligned} \tag{53}$$

are determined. Using Theorem 6 this data can be used to determine (a_2, b_2), the scattering data for $q_2 = \chi_{[t_-^{(1)}, t_+^{(1)}]} q$.

The method is applied iteratively to obtain sequences

$$t_-^{(0)} < \dots t_-^{(j)} < t_-^{(j+1)} < \dots < t_+^{(j+1)} < t_+^{(j)} < \dots t_+^{(0)}.$$

In the Appendix A we show that, given sufficiently smooth initial data r there is $\Delta > 0$ so that, for all $j \geq 0$,

$$|t_\pm^{(j)} - t_\pm^{(j+1)}| > \Delta.$$

Hence after finitely many steps the potential q is determined on the whole real line.

We close this section by stating our algorithm as a sequence of steps. In the next section we indicate the modifications needed to handle the possible occurence of bound states for the "intermediate" potentials $\{q_j\}$.

STEP 0:

Solve the left and right Marchenko equations by iteration on "maximal" intervals $(-\infty, t_-^{(0)}]$, $[t_+^{(0)}, \infty)$. If $t_-^{(0)} \geq t_+^{(0)}$ we are done. Otherwise determine the scattering data for $q_-^{(0)}$ and $q_+^{(0)}$. Apply Theorem 6 to determine the scattering data for q_1. Set $j = 1$ and proceed to step 1.

STEP 1:

Use the reflection coefficient for q_j in (52) to determine the kernel function f_j (g_j) supported on $(-\infty, 2t_+^{(j-1)}]$ ($[2t_-^{(j-1)}, \infty)$).

STEP 2:

Solve the Marchenko equation on the interval $[t_+^{(j)}, t_+^{(j-1)}]$ ($[t_-^{(j-1)}, t_-^{(j)}]$). If $t_-^{(j)} \geq t_+^{(j)}$ we are done, otherwise go to step 3.

STEP 3:

Determine the scattering data, on the real line for the potentials

$$q_-^{(j)} = \chi_{[t_-^{(j-1)}, t_-^{(j)}]} q, \quad q_+^{(j)} = \chi_{[t_+^{(j)}, t_+^{(j-1)}]} q$$

and apply Theorem 6 to determine the scattering data, on the real line, for

$$q_{j+1} = \chi_{[t_-^{(j)}, t_+^{(j)}]} q.$$

STEP 4: Go to step 1 with j replaced by j+1.

6 What is time?

Before we turn to the computation of examples we need to consider the physical significance of the t-parameter which appears in (11). This is intimately connected to the problem of rephasing. The main clue comes from (35). Suppose that q is a potential supported in $[t_0, t_1]$ with reflection coefficient r. After time $= t_1$ a solution to (11) is freely precessing in the local (gradient offset) B_0-field.

If $t_1 = 0$ then, at the end of the RF-excitation, the magnetization satisfies

$$\frac{(m_{11-} + im_{21-})(\xi; 0)}{1 + m_{31-}(\xi; 0)} = r(\xi). \tag{54}$$

We have therefore achieved the desired magnetization profile without any need for rephasing. If on the other hand $t_1 < 0$ then, at the end of the excitation, the magnetization satisfies

$$\frac{(m_{11-} + im_{21-})(\xi; t_1)}{1 + m_{31-}(\xi; t_1)} = e^{2i\xi t_1} r(\xi). \tag{55}$$

In order to get the desired magnetization profile the spins must freely precess for $|t_1|$-units of time. Finally if $t_1 > 0$ then the spins must precess for $-t_1$-units of time. In other words either a 180°-refocussing pulse must be applied or the gradient needs to be reversed, followed by t_1-units of free precesion, in order to achieve the magnetization profile specifed by r.

In RF-pulse synthesis the data is specified in the *frequency* domain. Given $r(\xi)$ and perhaps some bound states $\{(\xi_j, C_j)\}$ the IST produces a potential which is a function of t. The support of this potential is determined by the scattering data and thereby determines what sort of rephasing is needed to achieve the specified magnetization profile. If the *essential* support of the potential is contained in $[t_0, t_1]$ then, according to the sign of t_1, the necessary rephasing is determined as in the previous paragraph. The main point to note is that the time dependence of the potential is an *output* of the IST. In particular, the numerical value of t_1, in appropriate units, determines the rephasing which is needed to achieve the specified magnetization profile. When computing the total energy requirement for an RF-envelope with $t_1 > 0$ one must include the energy of the (hard) 180°-pulse or that of transients produced by reversing the gradient.

Two tools are available to manipulate the support of q. On the one hand we can use smooth approximations to r so that its Fourier transform is rapidly decreasing. The estimate (46) shows that this reduces the essential support of q. The other tool is the introduction of bound states, coupled with methods of meromorphic approximation. Rourke and Morris approximate r by rational functions which decay at infinity and obtain potentials with support in $(-\infty, 0]$. The rational approximations to r which they use have poles in the upper half plane and these in turn lead to an increase in the energy and the oscillation of the RF-envelope. This is the price for an envelope that does not require rephasing. For the standard pulses used in MR imaging the minimum energy pulse in general requires rephasing.

The problem of finding approximations that carefully balance the rephasing requirements with the energy of the pulse itself seems a very interesting field for further investigation. Through the Marchenko equations and the Paley-Wiener Theorem II it translates to the problem of approximating the function r, defined on real axis, by meromorphic functions ρ, defined in the upper half plane, which satisfy an estimate of the form

$$\int_{-\infty}^{\infty} e^{-4\eta T} |\rho(\xi + i\eta)|^2 d\xi \leq C \text{ for } \eta \geq 0.$$

Here C and T are positive constants. The resultant potential will be supported in $(-\infty, T]$. We will return to this variational problem in a subsequent publication.

7 Examples

8 Analysis of the hard pulse approximation

The Shinnar-Le Roux algorithm uses the *hard pulse approximation* to design an RF-envelope. Given a magnetization profile $r(\xi)$ the SLR-algorithm designs a potential of the form

$$q_0 = \sum_{j=1}^{N} \mu_j \delta(t - j\Delta),$$

to produce a good approximation to the desired profile over a sub-interval of

$$[-\Delta^{-1}\pi, \Delta^{-1}\pi].$$

The reflection coefficient, r_0 defined by q_0 is a *periodic* function of period $\Delta^{-1}2\pi$. The SLR-algorithm provides an iterative method for determining the coefficients $\{\mu_j\}$.

Of course a sum of δ-pulses is non-physical, requiring infinite energy to realize. The RF-envelope which is actually used is a "softened" version of q_0. For example one could replace each $\mu_j \delta(t - j\Delta)$ by a boxcar pulse of width Δ with the same area, leading to the softened pulse:

$$q_1 = \sum_{j=1}^{N} \frac{\mu_j}{\Delta} \chi_{[0,\Delta)}(t - j\Delta),$$

see [14]. There is no reasonable sense in which the difference $q_0 - q_1$ is "small." Nonetheless, under certain conditions, the difference $|r_0(\xi) - r_1(\xi)|$ can be made small for ξ in fixed interval. The reflection coefficient, r_1 corresponding to q_1 tends to zero at infinity. The relationship between r_0 and r_1 is studied below.

The SLR approach should be contrasted with the approach outlined above: Given r we approximate it by a smooth magnetization profile r_s. We then construct a smooth potential q_s with reflection coefficient r_s. Such a pulse is again implemented by replacing it with a sum like q_1. So there should be no confusion, we denote a sequence of boxcar pulses approximating q_s by q_{s1}. Below we show that the difference in the magnetization profile produced by q_s and that produced by q_{s1} is controlled by $\|q_{s1} - q_s\|_{L^1}$.

For our analysis of the hard pulse approximation we consider the one parameter family of pulses

$$q_\epsilon = \sum_{j=1}^{N} \frac{\mu_j}{\epsilon\Delta} \chi_{[0,\epsilon\Delta)}(t - j\Delta), \quad \epsilon \in [0, 1], \tag{56}$$

with the understanding that q_0 is the sum of δ-pulses given above. It is a simple computation to show that

$$\int_{-\infty}^{\infty} |q_\epsilon(t)| dt$$

is independent of ϵ and

$$\int_{-\infty}^{\infty} |q_\epsilon(t)|^2 dt = \frac{1}{\epsilon} \int_{-\infty}^{\infty} |q_1(t)|^2 dt.$$

This formula indicates the desirability of using q_1 to approximate q_0 rather than q_ϵ for an $\epsilon < 1$.

Let r_ϵ denote the reflection coefficient defined by q. The potential q_ϵ is supported in the interval $[0, N\Delta]$. In order to study r_ϵ we need to find a formula for $\psi_{\epsilon 1-}(\xi; N\Delta)$. As is well known, this can be conveniently expressed in terms of a product of 2×2-matrices. The solution operator at time $t_0 + \Delta$ to the ZS-system with potential given by

$$\epsilon^{-1}\mu\chi_{[0,\epsilon\Delta)}(t - t_0)$$

is

$$U_{\mu,\epsilon,\Delta}(\xi) = \begin{bmatrix} e^{-i(1-\epsilon)\Delta\xi}\left(\cos(\alpha) - \frac{i\epsilon\Delta\xi\sin(\alpha)}{\alpha}\right) & e^{-i(1-\epsilon)\Delta\xi}\left(\frac{i\mu\sin(\alpha)}{\alpha}\right) \\ e^{i(1-\epsilon)\Delta\xi}\left(\frac{i\mu^*\sin(\alpha)}{\alpha}\right) & e^{i(1-\epsilon)\Delta\xi}\left(\cos(\alpha) + \frac{i\epsilon\Delta\xi\sin(\alpha)}{\alpha}\right) \end{bmatrix}, \tag{57}$$

where

$$\alpha = \sqrt{\xi^2 + |\mu|^2}. \tag{58}$$

The solution operator for the ZS-system, at time $N\Delta$ with the potential given by (56) is therefore the product of the 2×2-matrices:

$$\begin{aligned} U_{\epsilon,\Delta}(\xi) &= U_{\mu_N,\epsilon,\Delta}(\xi) \cdots U_{\mu_1,\epsilon,\Delta}(\xi) \\ &\doteq \begin{bmatrix} A_\epsilon(\xi) & -B_\epsilon^*(\xi) \\ B_\epsilon(\xi) & A_\epsilon^*(\xi) \end{bmatrix}. \end{aligned} \tag{59}$$

It follows easily from (34) that

$$r_\epsilon(\xi) = \frac{B_\epsilon(\xi)e^{-2iN\Delta\xi}}{A_\epsilon(\xi)}. \tag{60}$$

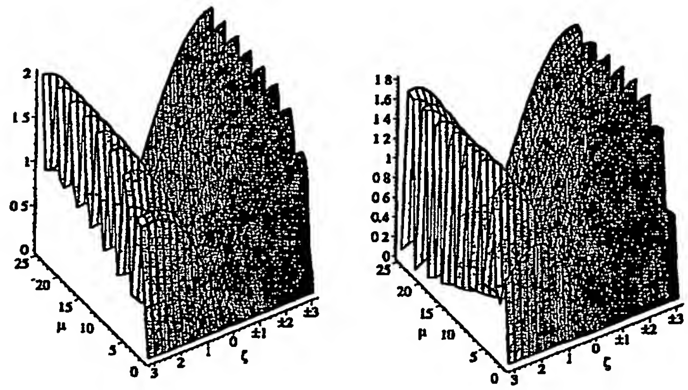
The entries of (57), (59) and (57) are are continuous at $\epsilon = 0$. The functions (A_ϵ, B_ϵ) are the scattering coefficients for the ZS-system with potential q_ϵ. If $\epsilon \neq 0$ the asymptotics established in (65) are applicable. If $\epsilon = 0$ then A_0 and B_0 can be expressed as

$$A_0(\xi) = e^{iM\Delta\xi} P(e^{i\Delta\xi}), \quad B_0(\xi) = e^{iM'\Delta\xi} Q(e^{i\Delta\xi}),$$

Where P and Q are polynomials of degree $N - 1$. As expected A_0 and B_0 are $\Delta^{-1}2\pi$-periodic functions.

The SLR design process begins with $r_0(\xi)$, a rational function of an appropriate degree in $e^{i\Delta\xi}$, approximating the desired magnetization profile $r(\xi)$ over the interval $[-\Delta^{-1}\pi, \Delta^{-1}\pi]$. The algorithm then determines coefficients $\{\mu_j\}$ so that

$$r_0(\xi) \approx \frac{B_0(\xi)e^{-2iN\Delta\xi}}{A_0(\xi)}.$$



(a) A plot of D_1.

(b) A plot of D_2.

Figure 1: Plots of the error functions D_1 and D_2 for $\mu \in [0, 25]$.

As with the IST approach this problem does not have a unique solution. The different solutions are labeled, in essence, by the locations of the zeros of P outside the unit disk. These correspond to zeros of A_0 in the upper half plane. The questions of principal interest are:

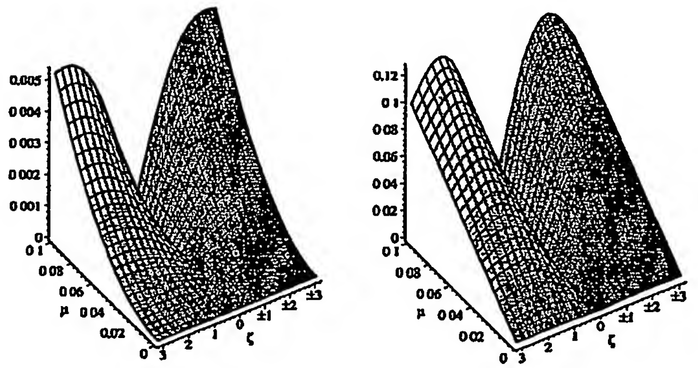
1. How well does $r_1(\xi)$ approximate $r_0(\xi)$ over the interval $[-\Delta^{-1}\pi, \Delta^{-1}\pi]$?
2. How rapidly does r_1 decay outside of $[-\Delta^{-1}\pi, \Delta^{-1}\pi]$?
3. How are the zeros of A_1 in the upper half plane related to those of A_0?

The first question admits of a fairly simple analysis. We first consider a single term in the product expansion (59), examining the dependence of the difference $\|U_{\mu,1,\Delta}(\xi) - U_{\mu,0,\Delta}(\xi)\|$ on (μ, Δ) for ξ in the interval $[-\Delta^{-1}\pi, \Delta^{-1}\pi]$. By setting $\zeta = \Delta\xi$ this reduces to consideration of the differences

$$\begin{aligned} D_1(\mu,\zeta) &= \left| e^{i\zeta}\left(\cos\sqrt{|\mu|^2+\zeta^2} - \frac{i\zeta\sin\sqrt{|\mu|^2+\zeta^2}}{\sqrt{|\mu|^2+\zeta^2}}\right) - \cos|\mu| \right| \\ D_2(\mu,\zeta) &= \left| \frac{\mu\sin\sqrt{|\mu|^2+\zeta^2}}{\sqrt{|\mu|^2+\zeta^2}} - \frac{\mu\sin|\mu|}{|\mu|} \right|, \end{aligned} \tag{61}$$

for $\zeta \in [-\pi, \pi]$. As the plots in figures 1 and 2 show, the only way to make both differences small is to take $|\mu|$ small.

In terms of pulse design, this means that Δ should be taken to be small which in



(a) A plot of D_1. (b) A plot of D_2.

Figure 2: Plots of the error functions D_1 and D_2 for $\mu \in [0, 0.1]$.

turn forces N to be large. A computation with Taylor series shows that

$$\begin{aligned} D_1(\mu, \zeta) &= |\mu|^2 F(\mu, \zeta), \\ D_2(\mu, \zeta) &= |\mu|(|\mu|^2 G(\mu, \zeta) + \zeta^2 H(\zeta^2), \end{aligned} \tag{62}$$

here F, G, H are entire functions. For a fixed target magnetization r the $\{\mu_j\}$ appearing in (59) satisfy

$$|\mu_j| = O(\Delta) = O(N^{-1}).$$

For ξ restricted to a *fixed* finite interval, ζ also behaves like $O(N^{-1})$. With this restriction on ξ both error functions behave like $O(N^{-2})$ as N tends to infinity.

We express $U_{1,\Delta}$ as

$$U_{1,\Delta} = U_{\mu_N,0,\Delta}(\mathrm{Id}_2 + E_N) U_{\mu_{N-1},0,\Delta}(\mathrm{Id}_2 + E_{N-1}) \cdots U_{\mu_1,0,\Delta}(\mathrm{Id}_2 + E_1),$$

where

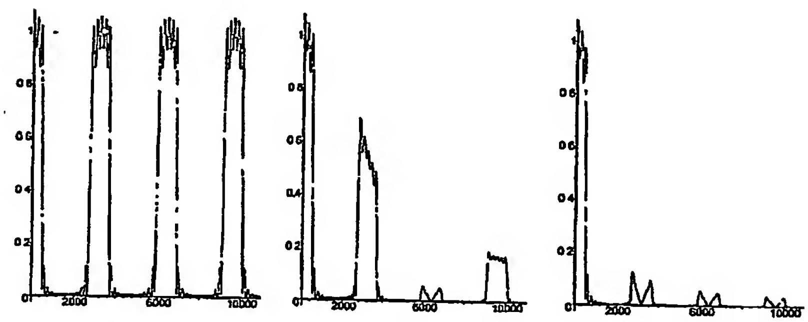
$$\mathrm{Id}_2 + E_j = U_{\mu_j,0,\Delta}^{-1} U_{\mu_j,1,\Delta}.$$

Using this expression and the estimates above one can show that the differences

$$|A_1(\xi) - A_0(\xi)|, \quad |B_1(\xi) - B_0(\xi)|$$

can be made uniformly $O(N^{-1})$ for ξ belonging to a fixed interval, provided N is sufficiently large. Note that if the error in the individual terms were of order N^{-1} then this statement would not be true, as indicated by the well known formula

$$\lim_{N\to\infty} \left(1 + \frac{1}{N}\right)^N = e.$$



(a) A plot of $|r_0|$, the hard pulse approximation.

(b) A plot of $|r_{\frac{1}{2}}|$, an intermediate case.

(c) A plot of $|r_1|$, the soft pulse approximation.

Figure 3: Plots of the absolute magnetization profi les for various approximations to a 90°-sinc pulse showing several fundamental periods.

Thus by taking N large and therefore Δ small the softened SLR pulse should provide a good approximation to the desired magnetization over a fi xed interval where A_0 does not vanish. For a fi xed N the behavior of $\eta(\xi)$ for large $|\xi|$ is governed by (65). Empirically it is well known that r_1 is quite small outside of $[-\Delta^{-1}\pi, \Delta^{-1}\pi]$. The plots in fi gure 3 shows the magnitude of the magnetization profi les for several approximations to a 90°-sinc-pulse with a bandwidth of 1000Hz. Note that $r_{\frac{1}{2}}$ has considrable support outside the fundamental period $[-500, 500]$.

The answer to the last question is not immediately clear. According to [10], the minimum energy *SLR pulse* is attained by placing all the roots of P inside the unit circle. This accords well with our analysis, as it is zeros of a in the upper half plane, which corresponds to the exterior of the unit circle, that increase the energy requirements of an RF-envelope. The asymptotic analysis above shows that zeros of A_0 in the upper half plane that are close to the real segment $[-\Delta^{-1}\pi, \Delta^{-1}\pi]$ are likely to produce zeros of A_1 in the upper half plane which thereby increase the energy requirement of the softened pulse. The behavior of the zeros of A_ϵ as ϵ goes from 0 to 1 seems an interesting question for further investigation.

By way of contrast, using the IST method one is in direct control of the zeros of a in the upper half plane as well as the phase of the magnetization profi le. We close this section by stating an estimate which shows that replacing the smooth RF-envelope found using the IST by a soft pulse approximation q_{s1} does not result in substantial errors in the magnetization profi le.

Theorem 8. *Suppose that h_1 and h_2 are integrable potentials for the ZS-system, and*

that $F_i^{\pm}(\xi), i = 1, 2$ solves the ZS-system with potential $h_i, i = 1, 2$. Let

$$\begin{aligned} H^-(t) &= \int_{-\infty}^{t} |h_1(s) - h_2(s)|ds, \quad Q^-(t) = \int_{-\infty}^{t} |h_1(s)|ds, \\ H^+(t) &= \int_{t}^{\infty} |h_1(s) - h_2(s)|ds, \quad Q^+(t) = \int_{t}^{\infty} |h_1(s)|ds. \end{aligned} \tag{63}$$

If

$$\lim_{t\to\pm\infty} \|F_1^{\pm}(\xi;t) - F_2^{\pm}(\xi;t)\| = 0.$$

then, for $\xi \in \mathbb{R}$ the differences satisfy the estimates

$$\|F_1^{\pm}(\xi;t) - F_2^{\pm}(\xi;t)\| \leq 2I_0(2\|h_2\|_{L^1})H^{\pm}(t)\exp(Q^{\pm}(t)). \tag{64}$$

The proof is in Appendix B.

In light of these estimates it is clear that by choosing a soft approximation q_{s1} to the smooth pulse q_s so that $\|q_s - q_{s1}\|_{L^1}$ is small, the reflection coefficient r_{s1} can be made uniformly close to r_s over any desired interval where a_s does not vanish. Once again this amounts to using a small value of Δ in the definition of q_{s1}.

9 Appendices

9.1 Appendix A: Solving the Marchenko equation II

We now explain the modifications to the algorithm presented in section 5 which are required if the intermediate potentials $\{q_j\}$ have non-trivial bound states. Suppose that φ is a function with two continuous derivatives and $-\infty < \alpha < \beta < \infty$. In Appendix B we establish the following asymptotic formulæ and estimates for the scattering data (a_c, b_c) for the ZS-system with potential $\chi_{[\alpha,\beta]}\varphi$:

$$\begin{aligned} a_c(\xi) &= 1 + \frac{\|\varphi\|^2_{L^2[\alpha,\beta]}}{2i\xi} + O\left(\frac{1}{(1+|\xi|)^2}\right), \\ e^{2i\xi\beta} b_c(\xi) &= e^{2i\xi\beta}\hat{T}_{[\alpha,\beta;\varphi^*(\alpha),\varphi^*(\beta)]}(2\xi) + O\left(\frac{1}{(1+|\xi|)^2}\right). \end{aligned} \tag{65}$$

Here $T_{[\mu,\nu;A,B]}$ is the piecewise, linear function

$$T_{[\mu,\nu;A,B]}(t) = \chi_{[\mu,\nu]}(t)\frac{B(t-\mu) + A(\nu - t)}{\nu - \mu}. \tag{66}$$

These formulæ hold uniformly in the upper half plane with the implied constants in the O-terms bounded in terms of the $\mathcal{C}^2([\alpha,\beta])$-norm of φ. The formula for a_c shows that the zeros of this function, in the upper half plane are constrained to lie in a fixed ball

of radius R_0. Dividing these formulæ gives an asymptotic formula and estimate for the reflection coefficient, r_c :

$$e^{2i\xi\beta}r_c(\xi) = e^{2i\xi\beta}\hat{T}_{[\alpha,\beta;\varphi^*(\alpha),\varphi^*(\beta)]}(2\xi) + O\left(\frac{1}{(1+|\xi|)^2}\right). \tag{67}$$

The error term in again uniformly estimated in the upper half plane outside the ball of radius $R_0 + 1$ (say). Observe that both r_c and $\partial_\xi r_c$ belong to $L^2(\mathbb{R})$. Thus the results of Beals and Coifman show that the inverse scattering transform can be applied to this data.

We can now complete the proof of Theorem (7)

Proof of Theorem (7). If q has support in $(-\infty, t_+]$ then the scattering coefficient b has an analytic extension to the upper half plane. This is because $\psi_{1+} = [e^{-i\xi t}, 0]^\dagger$ for $t \geq t_+$ and therefore equation (22) shows that

$$b(\xi) = \psi_{21-}(\xi; t_+)e^{-i\xi t_+}.$$

If r has a meromorphic extension to the upper half plane then the integrand in the Marchenko equation, defined in (36), has a different representation. If the zeros of a in the upper half plane have imaginary parts less than η_0 then

$$f(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{b(\xi + i\eta_0)}{a(\xi + i\eta_0)} e^{i(\xi+i\eta_0)t} d\xi, \tag{68}$$

see [1]. Provided that the potential has support in a positive half line, there is an analogous formula expressing g, the kernel function in the left Marchenko, as an integral over the line $\{\xi - i\eta_0 \,:\, \eta_0 \in \mathbb{R}\}$:

$$g(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{b^*(\xi - i\eta_0)}{a(\xi - i\eta_0)} e^{-i(\xi-i\eta_0)t} d\xi. \tag{69}$$

Using the asymptotic formula given in (65) and the asymptotics for ψ_{21-} that follow from (16) and (18), we conclude that $e^{2i\xi t_+}r$ satisfies the hypotheses of the Paley-Wiener Theorem II in the half plane $\operatorname{Im}\xi \geq \eta_0$ (see Appendix B). This function is therefore the Fourier transform of a function with support in $(-\infty, 0]$. Hence f is supported in $(-\infty, 2t_+]$. This argument applies *mutatis mutandis* to the kernel of the left Marchenko equation. □

Remark 9. If a has only simple zeros then (68) implies that the norming constants are given by

$$C_i = \frac{b(\xi_i)}{a'(\xi_i)}.$$

There is a similar formula for the $\{\widetilde{C}_i\}$. Given that the potential has support in an appropriate half line, the formulæ (68) and (69) define the kernel functions for the Marchenko equation whether or not the zeros of a are simple.

Since the potentials $\{q_j\}$ have bounded support and q is assumed to have at least two derivatives the estimates in (65) apply for each $j \geq 1$. The scattering coeffi cients $\{(a_j, b_j)\}$ are entire functions. The asymtptotic formula for a_j implies that is has at most fi nitely zeros in the upper half plane. Denote these zeros by $\{\xi_i^{(j)} : i = 1, \ldots, N_j\}$ At step j we have determined

$$\tilde{q}_j = \chi_{(-\infty, t_-^{(j-1)}]} q + \chi_{[t_+^{(j-1)}, \infty)} q.$$

Equation (39) implies that

$$\int_{-\infty}^{\infty} |q(t)|^2 dt = \frac{1}{\pi} \int_{-\infty}^{\infty} \log(1 + |r(\xi)|^2) d\xi.$$

It is not diffi cult to show that (39) can be extended to potentials of the form $\chi_{[\alpha,\beta]} q$, with q twice differentiable, so that:

$$\int_{-\infty}^{\infty} |q_j(t)|^2 dt = \frac{1}{\pi} \int_{-\infty}^{\infty} \log(1 + |r_j(\xi)|^2) d\xi + 4 \sum_{l=1}^{N_j} \operatorname{Im} \xi_l^{(j)}.$$

Using these formulæ gives

$$4 \sum_{i=1}^{N_j} \operatorname{Im} \xi_i^{(j)} = \frac{1}{\pi} \int_{-\infty}^{\infty} \log\left(\frac{1 + |r(\xi)|^2}{1 + |r_j(\xi)|^2}\right) d\xi - \int_{-\infty}^{\infty} |\tilde{q}_j(t)|^2 dt. \tag{70}$$

This relation gives an upper bound on the imaginary part of any root of a_j :

$$\begin{aligned} 4 \operatorname{Im}(\xi_i^{(j)}) &\leq \frac{1}{\pi} \int_{-\infty}^{\infty} \log\left(\frac{1 + |r(\xi)|^2}{1 + |r_j(\xi)|^2}\right) d\xi - \int_{-\infty}^{\infty} |\tilde{q}_j(t)|^2 dt \\ &\leq \int_{-\infty}^{\infty} |q(t)|^2 dt. \end{aligned} \tag{71}$$

We fi x η_0 to be a non-negative number, larger than $\max_{i,j} \{\operatorname{Im} \xi_i^{(j)}\}$ or zero if this maximum is zero.

In light of the upper bound (71) on the imaginary parts of the zeros of the functions $\{a_j\}$, we can use the estimates in (65) to further conclude that the integrands $\{f_j : j \geq 1\}$ are uniformly bounded in $[2t_-^{(j-1)}, 2t_+^{(j-1)}]$. Indeed each is the sum of a piecewise linear function of the type defi ned in (66) and a continuous function with support in $(-\infty, 2t_+^{(j-1)}]$ which vanishes at $-\infty$. In light of Theorem 5 this establishes the claim, made in section 5, that there is a $\Delta > 0$ so that

$$|t_\pm^{(j)} - t_\pm^{(j-1)}| > \Delta.$$

These observations show that the algorithm in section 5 applies to the case where the intermediate potentials have bound states so long as we use (68) ((69)) to compute the $\{f_j\}$ ($\{g_j\}$). This formula requires the analytic continuation of the scattering data into the upper half plane. Since we know, *a priori* that a_j and b_j have such extensions, the estimates in (65) apply to show that the Cauchy integral formula gives:

$$\begin{aligned} a_j(\xi + i\eta) &= 1 + \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{(a_j(\zeta) - 1)d\zeta}{\zeta - (\xi + i\eta)}, \\ b_j(\xi + i\eta) &= \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{b_j(\zeta)d\zeta}{\zeta - (\xi + i\eta)}. \end{aligned} \tag{72}$$

To obtain an algorithm that succeeds in solving the Marchenko equations in all cases we need only modify Step 1 in the earlier algorithm:

STEP 1': Use (28) to determine if the reflection coeffi cient for q_j has poles in the upper half plane. If so extend (a_j, b_j) to the line $\operatorname{Im}\xi = \eta_0$ and use (68) ((69)) to determine the kernel function(s) f_j (g_j) supported in the ray $(-\infty, 2t_+^{(j-1)}]$ ($[2t_-^{(j-1)}, \infty)$).

We close this appendix with some remarks on the implementation of this algorithm.

1. It is well known that it is not necessary to solve the 2×2-matrix system (37) to fi nd $\mathcal{K}_{12t}$. By substitution this can be reduced to solving a scalar integral equation, see [1].

2. Given that the initial data r (or m^{∞}) is assumed to be smooth, with bounded support there is no problem, in principle, in determining $q_{\pm}^{(0)}$. The scattering data for these potentials can be determined by numerically solving the ZS-system with the given potentials. The method used in section 8 gives alternate algebraic approach to the approximate determination of the scattering coeffi cients.

3. In the subsequent steps of the algorithm we are working with potentials with bounded support but jump discontinuities. The diffi culties that this might engender, like the Gibbs phenomenon, can be avoided by using the asymptotic expansion (67) in (68). That is, we set

$$\check{r}_j(\xi) = r_j(\xi) - \hat{T}_{[t_-^{(j-1)}, t_+^{(j-1)}; q^*(t_-^{(j-1)}), q^*(t_+^{(j-1)})]}(2\xi).$$

The contribution of $\hat{T}_{[t_-^{(j-1)}, t_+^{(j-1)}; q^*(t_-^{(j-1)}), q^*(t_+^{(j-1)})]}$ to f_j can be exactly determined. It is a function with support in $[2t_-^{(j-1)}, 2t_+^{(j-1)}]$. The function $\check{r}_j$ is $O(|\xi|^{-2})$ as $|\xi|$ goes to infi nity. This estimate holds uniformly in strips with bounded imaginary part in the upper half space. Thus in the computation of the approximate Fourier inverses

$$\frac{1}{2\pi}\int_{-R}^{R} r_j(\xi + i\eta_0)e^{i(\xi + i\eta_0)t}d\xi$$

we can avoid bothersome Gibbs-type artifacts. If q is smooth then there is a complete asymptotic expansion for each r_j which only depends on the (in principle known) values of the derivatives $\{q^{[k]}(t_{\pm}^{(j-1)})\}$. Using further terms in this expansion can produce even more rapidly convergent correction terms. This should be done with care as it requires the computation of derivatives of q which could in turn lead to numerical instability.

4. After Step 0 we are looking for spatially limited potentials. The input data for Step 1 is essentially in the frequency domain. Since we know $[t_{-}^{(0)}, t_{+}^{(0)}]$ we can choose the sample spacing in the frequency domain so as to avoid aliasing errors in the construction of these potentials.

5. The Cauchy integral in (72) is a shift invariant filter with transfer function $2\pi i\chi_{(-\infty,0]}(t)e^{t\eta}$. As such it is easily implemented in practice.

6. After a potential q with reflection coefficient r and no bound states is found, it is a relatively simple matter to add in bound states. An algorithm to do this is described in section 6 of [3]. One possible usage for bound states is to reduce the effective support of the potential. To that end one might chose points $\{\xi_1, \ldots, \xi_N\}$ in the upper half plane and norming constants $\{C_j\}$ so that sum

$$i\sum_{j=1}^{N} C_j e^{i\xi_j t}$$

approximates

$$\check{r}(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} r(\xi)e^{i\xi t}d\xi$$

over some ray $[T, \infty)$. With these choices the effective support of f defined in (36) can be made smaller than that of $\check{r}$ and thereby a potential with smaller (effective) support, producing the same magnetization profile can be found. This is of course at the expense of

$$4\sum_{j=1}^{N} \operatorname{Im}\xi_j$$

in additional energy. In section 6 we saw that the effective support of q determines the rephasing which is needed to obtain the specified magentization profile.

7. While the bound states do not affect the observable magnetization they do affect the spins themselves. Bound states might prove useful in designing pulse sequences intended to manipulate higher order quantum coherences.

8. The computation in (28) has an integer valued result. Using the asymptotic

formula (65) it is not difficult to give an estimate for R so that the finite integral

$$\int_{-R}^{R} \frac{a_j'(\xi)d\xi}{a_j(\xi)\cdot(2\pi i)}$$

suffices to determine N_j.

9.2 Appendix B: Mathematical proofs

The Paley-Wiener Theorems: The "Paley-Wiener" Theorem is used several times in this paper. This is really a collection of results relating the support properties of a function defined on $\mathbb{R}$ to the analytic continuation of its Fourier transform. A complete discussion can be found in [17]. Two results adequate for our applications are:

Theorem 9 (Paley-Wiener Theorem I). *A function f in $L^2(\mathbb{R})$ has bounded support in the interval $[-L, L]$ if and only if its Fourier transform has an analytic extension to the entire complex plane satisfying:*

$$|\hat{f}(\xi + i\eta)| \leq Ce^{L|\eta|}, \tag{73}$$

for a constant C.

and

Theorem 10 (Paley-Wiener Theorem II). *A function f in $L^2(\mathbb{R})$ has support in the ray $(-\infty, 0]$ if and only if its Fourier transform has an analytic extension to the upper half plane satisfying*

$$\begin{aligned} &\int_{-\infty}^{\infty} |\hat{f}(\xi + i\eta)|^2 \leq C \textit{ and} \\ &\lim_{\eta\downarrow 0} \int_{-\infty}^{\infty} |\hat{f}(\xi + i\eta) - \hat{f}(\xi)|^2 = 0. \end{aligned} \tag{74}$$

The proof of Theorem 5: Assuming that $I_f(2t) < 1$ We need to show that the Marchenko equation,

$$\mathcal{K}_t(s) - \int_t^{\infty} \mathcal{K}_t(s+x)\mathcal{F}(t+x)dx = -\mathcal{F}(s+t), \tag{75}$$

can be solved by the iteration defined in (44) and the solution satisfies the estimate in (45). The proof is a simple induction argument. Clearly $|||\mathcal{K}_t^0(s)||| \leq M_f(t+s)$. Assume that

$$\left|\left|\left|\mathcal{K}_t^j(s)\right|\right|\right| \leq M_f(t+s)\left[1 + I_f(2t) + \ldots I_f^j(2t)\right]. \tag{76}$$

It follows from this assumption that

$$\left|\left|\left|\mathcal{K}_t^{j+1}(s)\right|\right|\right| \leq M_f(t+s) + \left[1 + I_f(2t) + \dots I_f^j(2t)\right] \times \int_t^{\infty} M_f(t+x)\|\mathcal{F}(t+x)\|dx.$$

The induction hypothesis (76), with j replaced by $j+1$ follows easily from this estimate. Using a similar argument we can show that, for $j \geq 1$

$$\left|\left|\left|\mathcal{K}_t^j(s) - \mathcal{K}_t^{j-1}(s)\right|\right|\right| \leq M_f(t+s)I_f(2t)^j \tag{77}$$

If $I_f(2t) < 1$ then this estimate shows that $\{\mathcal{K}_t^j\}$ is a uniformly convergent sequence for $s \in [t, \infty)$. The limit, $\mathcal{K}_t^{\infty}$ is evidently a solution to (75). We can also pass to the limit in (76) to conclude that $\mathcal{K}_t^{\infty}$ satisfi es (45).

The proof of (65): We use the integral equations (16) defi ning the components of ψ_{1-}. Let

$$f_1(\xi; t) = \psi_{11-}(\xi; t)e^{i\xi t}.$$

It follows from (15), (16) and (19) that

$$\begin{aligned} a_c(\xi) &= 1 + \int_{\alpha}^{\beta} M_1(\xi; \infty, s) f_1(\xi; s) ds, \\ b_c(\xi) &= -\int_{\alpha}^{\beta} e^{-2i\xi s}\varphi^*(s) f_1(\xi; s) ds. \end{aligned} \tag{78}$$

In light of the simple form assumed by the potential we see, integrating by parts, that

$$\begin{aligned} M_1(\xi; \infty, s) &= -\varphi^*(s)\chi_{[\alpha,\beta]}(s) \int_s^{\beta} e^{2i\xi(x-s)}\varphi(x)dx \\ &= -\varphi^*(s)\chi_{[\alpha,\beta]}(s)\left[\frac{e^{2i\xi(\beta-s)}\varphi(\beta) - \varphi(s)}{2i\xi} - \int_s^{\beta} \frac{e^{2i\xi(x-s)}\varphi'(x)}{2i\xi}dx\right] \end{aligned} \tag{79}$$

Since $(x - s) \geq 0$, in the integral, this expression remains uniformly bounded for ξ in the upper half plane and implies that

$$M_1(\xi; \infty, s) = -\varphi^*(s)\chi_{[\alpha,\beta]}(s)\left[\frac{e^{2i\xi(\beta-s)}\varphi(\beta) - \varphi(s)}{2i\xi} + O\left(\frac{1}{1+|\xi|^2}\right)\right]. \tag{80}$$

This formula holds for ξ with non-negative real part with the implied constant in the O-term only depending on the $\mathcal{C}^2[\alpha, \beta]$-norm of φ.

Using this formula for $M_1(\xi;\infty,s)$ in (78) gives

$$\begin{aligned} a_c(\xi) &= 1+\frac{\|\varphi\chi_{[\alpha,\beta]}\|_{L^2}^2}{2i\xi}+O\left(\frac{1}{1+|\xi|^2}\right) \\ b_c(\xi) &= -\int_\alpha^\beta e^{-2i\xi s}\varphi^*(s)ds+O\left(\frac{1}{1+|\xi|^2}\right). \end{aligned} \tag{81}$$

This completes the analysis of a_c; for b_c we integrate by parts again to get:

$$b_c(\xi)=\frac{e^{-2i\xi\beta}\varphi^*(\beta)-e^{-2i\xi\alpha}\varphi^*(\alpha)}{2i\xi}+O\left(\frac{1}{1+|\xi|^2}\right). \tag{82}$$

The proof is completed by observing that

$$\hat{T}_{[\mu,\nu;A,B]}=-\frac{Be^{-i\nu\xi}-Ae^{-i\mu\xi}}{i\xi}+\frac{B-A}{\beta-\alpha}\frac{e^{-i\nu\xi}-e^{-i\mu\xi}}{\xi^2}.$$

If φ has $k+1$ derivatives then we can integrate by parts in (79) k-times to get an asymptotic expansion for M_1 with an error term of order $O(|\xi|^{-(k+1)})$. This can in turn be used in (16) and (78) to obtain higher order asymptotic expansions for a_c and b_c. For smooth potentials, vanishing at infi nity, expansions of this type are well known in the inverse scattering literature.

The proof of Theorem 8: The proof of this result is a small modifi cation of the proof of the estimate (18) given in [1]. Let σ denote the 2×2-matrix

$$\sigma=\begin{bmatrix}-1 & 0\\ 0 & 1\end{bmatrix}$$

and let

$$D^{\pm}(\xi;t)=e^{-it\xi\sigma}(F_1^{\pm}-F_2^{\pm}).$$

For real ξ and t the matrices $e^{\pm it\xi\sigma}$ are unitary and therefore

$$\|F_1^{\pm}-F_2^{\pm}\|=\|D^{\pm}\|.$$

The vector valued functions $D^{\pm}$ satisfy the equations

$$\begin{aligned} \partial_t D^{\pm} &= e^{-it\xi\sigma}\begin{bmatrix}0 & h_1\\ -h_1^* & 0\end{bmatrix}e^{it\xi\sigma}D^{\pm}+e^{-it\xi\sigma}\begin{bmatrix}0 & (h_1-h_2)\\ -(h_1^*-h_2^*) & 0\end{bmatrix}F_2^{\pm}. \\ \lim_{t\to\pm\infty} D^{\pm}(\xi;t) &= 0. \end{aligned} \tag{83}$$

We now restrict our attention to the $-$ case, the $+$ case is handled by an essentially identical argument.

The differential equation in (83) is equivalent to the integral equation

$$\begin{aligned} D^-(\xi;t) = &\int_{-\infty}^{t} e^{-is\xi\sigma}\begin{bmatrix} 0 & h_1(s) \\ -h_1^*(s) & 0\end{bmatrix} e^{is\xi\sigma} D^-(\xi;s)ds + \\ &\int_{-\infty}^{t} e^{-is\xi\sigma}\begin{bmatrix} 0 & (h_1-h_2)(s) \\ -(h_1^*-h_2^*)(s) & 0\end{bmatrix} F_2^-(s)ds. \end{aligned} \tag{84}$$

This is a Volterra equation which can be solved by the following iteration:

$$\begin{aligned} D_0^-(\xi;t) &= \int_{-\infty}^{t} e^{-is\xi\sigma}\begin{bmatrix} 0 & (h_1-h_2)(s) \\ -(h_1^*-h_2^*)(s) & 0\end{bmatrix} F_2^-(s)ds \\ D_j^-(\xi;t) &= D_0^-(\xi;t) + \int_{-\infty}^{t} e^{-is\xi\sigma}\begin{bmatrix} 0 & h_1(s) \\ -h_1^*(s) & 0\end{bmatrix} e^{is\xi\sigma} D_{j-1}^-(\xi;s)ds, \end{aligned} \tag{85}$$

for $j \geq 1$.

First observe that the operator norm defined by the Euclidean norm satisfies

$$\left\|\begin{bmatrix} 0 & \alpha \\ -\alpha^* & 0\end{bmatrix}\right\| = |\alpha|$$

and therefore (18) implies that

$$\|D_0^-(\xi;t)\| \leq 2I_0(\|h_2\|_{L^1})H^-(t);$$

we make the inductive assumption that

$$\|D_j^-(\xi;t)\| \leq 2I_0(\|h_2\|_{L^1})H^-(t)\left[\sum_{k=0}^{j}\frac{(Q^-(t))^k}{k!}\right]. \tag{86}$$

From these assumptions and (85) it follows that

$$\|D_{j+1}^-(\xi;t)\| \leq 2I_0(\|h_2\|_{L^1})\left(H^-(t) + \int_{-\infty}^{t}|h_1(s)|H^-(s)\left[\sum_{k=0}^{j}\frac{(Q^-(s))^k}{k!}\right]\right). \tag{87}$$

The definition of Q^- implies that

$$|h_1(s)| = \partial_s Q^-(s)$$

and therefore (87) implies that

$$\begin{aligned} \|D_{j+1}^-(\xi;t)\| &\leq 2I_0(\|h_2\|_{L^1})H^-(t)\left[1 + \int_{-\infty}^{t}\partial_s\left(\sum_{k=0}^{j}\frac{(Q^-(s))^{k+1}}{(k+1)!}\right)ds\right] \\ &= 2I_0(\|h_2\|_{L^1})H^-(t)\left(\sum_{k=0}^{j+1}\frac{(Q^-(s))^k}{k!}\right) \end{aligned} \tag{88}$$

thus completing the proof of the induction step. As

$$\lim_{J\to\infty} D_J^- = D^-,$$

letting J tend to infinity completes the proof of the theorem.

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I CLAIM:

1. A method of synthesizing minimum energy pulses for a given magnetization profile in a magnetic resonance imaging system, comprising the steps of:

determining minimum energy for an RF envelope producing the given magnetization profile;

using an inverse scattering transform to determine a minimum energy smooth pulse RF envelope that approximates the energy of said minimum energy RF envelope; and

generating pulses with energy that approximates said minimum energy smooth pulse RF envelope.

2. A method as in claim 1, comprising the step of determining auxiliary parameters including bound states and norming constants for reduced scattering data of a potential for the minimum energy used in said inverse scattering transform.

3. A method as in claim 1, wherein the energy required for the minimum energy smooth pulse RF envelope is independent of the phase of transverse magnetization.

4. A method as in claim 1, comprising the additional step of increasing the energy of the smooth pulse RF envelope in order to reduce rephrasing time.

5. A method as in claim 2, wherein the step of determining the minimum energy smooth pulse RF envelope comprises the step of solving left and right Marchenko equations by iteration on maximal intervals to determine the reduced scattering data and iteratively removing parts of the reduced scattering data produced by already known parts of the potential.

6. A method as in claim 1, comprising the step of replacing the smooth pulse RF envelope with a soft pulse approximation to said smooth pulse RF envelope.

7. A method of generating a desired frequency dependent excitation in a magnetic resonance imaging system using minimum energy selective RF pulses for a given magnetization profile corresponding to said desired frequency dependent

excitation, comprising the steps of:

determining minimum energy for an RF envelope producing the given magnetization profile;

using an inverse scattering transform to determine a minimum energy smooth pulse RF envelope that approximates the energy of said minimum energy RF envelope;

generating pulses with energy that approximates said minimum energy smooth pulse RF envelope; and.

applying the pulses to said magnetic resonance imaging system to obtain a desired selective excitation.